

Initial conditions for CDM particles and General Relativity

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We describe the irrotational dust component of the universe in terms of a relativistic gradient expansion and transform the resulting synchronous metric to a Newtonian coordinate system. The two metrics are connected via a space-like displacement field and a time-like perturbation, providing a relativistic generalization of the transformation from Lagrangian to Eulerian Coordinates. The relativistic part of the displacement field generates already at initial time a non-local density perturbation at second order. This is a purely relativistic effect since it originates from space-time mixing. We give two options, the passive and the active approach, on how to include the relativistic corrections for example in N -body simulations. In the passive approach we treat the corrections as a non-Gaussian modification of the initial Gaussian field (primordial non-Gaussianity could be incorporated as well). The induced non-Gaussianity depends on scale and the redshift at which initial conditions are set, with $f_{\text{NL}} \sim \text{few}$ for small enough scales and redshifts. In the active approach we show how to use the relativistic trajectory to obtain the initial displacement and velocity of particles for N -body simulations without modifying the initial Gaussian field.

I. INTRODUCTION

Linearized cosmological perturbation theory (CPT) is a key technique for studying the nature of cosmological inhomogeneities [1, 2]. Its extension to second order has been applied to: (1) inflation, together with the subsequent reheating [3–5], (2) to the coupled set of Einstein–Boltzmann equations of the primordial baryon–photon fluid [6–8], (3) to secondary effects after decoupling of the photons [9, 10], and (4) to late-time evolution of gravitational clustering [11, 12]. It is crucial to go to second order to understand non-linear aspects of the underlying physics, and to disentangle the various sources of non-Gaussianities.

Here we report a somewhat different source of non-Gaussianity, relevant for the initial conditions of the CDM cosmic component, which cannot be directly embedded into one of the above groups (1)–(4). Instead, non-Gaussianity arises because of the non-linear coordinate transformation from a synchronous metric akin to Lagrangian coordinates to a Newtonian-like coordinate system, used for example in setting up N -body simulations. In ref [13] it has been recently shown that such a coordinate transformation connects both metrics with a space-like displacement field and a time-like perturbation. The space-like displacement field is strongly related to the one in the Newtonian Lagrangian perturbation theory (LPT), and the time-like perturbation can be interpreted as the 3-velocity potential of the displacement field. This correspondence encourages us to interpret the synchronous coordinate system to be Lagrangian, attached to the CDM particles, whereas the observer’s

“Eulerian” position is at rest in the Newtonian frame. Indeed, the metric perturbations in the Newtonian frame resolve to the Newtonian cosmological potential in the appropriate limit.

Relativistic corrections in the displacement field should not influence the gravitational late-time evolution of the particle trajectories much. As we shall demonstrate however, the relativistic coordinate transformation leads to non-Gaussian contributions in the density perturbations, which relate to the 3-velocity potential of the displacement field. These corrections matter already at the initial time and can be interpreted as a non-Gaussian modification of an otherwise initial Gaussian field.

This *paper* is organized as follows. In section II we first present the gradient expansion metric in the synchronous frame for irrotational and pressureless cold dark matter (CDM) particles in a Λ CDM universe, where Λ denotes a cosmological constant. Then, we show how the residual freedom inherent in the gradient metric can be fixed, clarify its physical interpretation and separate the sources/origin of non-Gaussianities in the latter coordinate transformation, see section III. In section IV we interpret the relativistic corrections as the above mentioned non-Gaussian modification of the initial Gaussian field (“the passive approach”) and approximate them in terms of a bispectrum component; the particles are then displaced according to Newtonian LPT. In section V we describe the active approach where the initial Gaussian field is unaltered but the particles are displaced according to the relativistic trajectory. Then, in section VI we calculate the density contrast in the Newtonian coordinate system. Finally, we relate the density contrast in the Newtonian gauge to the one in N -body simulations (section VII), and we conclude in section VIII.

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II. THE GRADIENT EXPANSION METRIC

We use the gradient expansion technique to solve the Einstein equations [14–19], although related relativistic approximation schemes lead to similar results [20–22]. We use a comoving/synchronous line element

$$ds^2 = -dt^2 + \gamma_{ij}(t, \mathbf{q}) dq^i dq^j, \quad (1)$$

where t is the proper time of the CDM particles and \mathbf{q} are comoving/Lagrangian coordinates, constant for each pressureless and irrotational CDM fluid element. The gradient expansion approximates the spatial metric with a series containing an increasing number of spatial gradients expressed in powers of the initial Riemann 3-tensor and its spatial derivatives.¹ Assuming standard inflationary initial conditions, the initial seed metric is

$$k_{ij} = \delta_{ij} \left[1 + \frac{10}{3} \Phi(\mathbf{q}) \right], \quad (2)$$

where $\Phi(\mathbf{q})$ is the primordial Newtonian potential (in our case a Gaussian field), given at the initial time t_0 . Using the formalism of ref [13] we then obtain up to four spatial gradients²

$$\begin{aligned} \gamma_{ij}(t, \mathbf{q}) = a^2(t) & \left\{ \delta_{ij} \left(1 + \frac{10}{3} \Phi \right) \right. \\ & + 3D(t) \left[\Phi_{,ij} \left(1 - \frac{10}{3} \Phi \right) - 5\Phi_{,i}\Phi_{,j} + \frac{5}{6}\delta_{ij}\Phi_{,l}\Phi_{,l} \right] \\ & + \left(\frac{3}{2} \right)^2 E(t) \left[4\Phi_{,ll}\Phi_{,ij} - \delta_{ij}(\Phi_{,ll}\Phi_{,mm} - \Phi_{,lm}\Phi_{,lm}) \right] \\ & \left. + \left(\frac{3}{2} \right)^2 [D^2(t) - 4E(t)] \Phi_{,li}\Phi_{,lj} + \mathcal{O}(\Phi^3) \right\}, \quad (3) \end{aligned}$$

where “ $,i$ ” denotes a differentiation w.r.t. Lagrangian coordinate q_i , summation over repeated indices is implied, and we have defined ($\Lambda \neq 0$):

$$\begin{aligned} D(t) &= \frac{20}{9} \int^t \frac{dt'}{a^2(t')} J(t'), \\ E(t) &= \frac{200}{81} \int^t \frac{dt'}{a^2(t')} \left[\frac{K(t')}{a^2(t')} - \frac{9}{10} D(t') J(t') \right], \end{aligned} \quad (4)$$

with

$$\begin{aligned} J(t) &= [2a(t)]^{-1} \int^t a(t') dt', \\ K(t) &= a(t) \int^t a^{-1}(t') J^2(t') dt', \end{aligned} \quad (5)$$

with $a(t)$ the scale factor. This result is valid for Λ CDM. To keep expressions as simple as possible we treat the Einstein–de Sitter (EdS) universe in the following, i.e., $\Omega_m = 1$, $\Omega_\Lambda = 0$, and thus $a(t) = (t/t_0)^{2/3}$. We shall generalize our findings to Λ CDM later.

The precise limits in the above time-integrations mirror the chosen initial conditions which can be arbitrary. As we shall soon see the coefficients D and E give the time evolution of the displacement at linear and second-order respectively, and the velocity time coefficients are proportional to the time derivative of D and E . We thus need two constraints at any order, e.g., one for the initial displacement and the other for the initial velocity (alternatively one could replace one of them with the initial acceleration field). To get the constraint for the displacement we require at initial time

$$\lim_{t \rightarrow t_0} \gamma_{ij}(t, \mathbf{q}) = k_{ij}. \quad (6)$$

This can be only achieved if $D(t_0) = E(t_0) = 0$, as can be easily verified through eq. (3). As we shall see the vanishing displacement field at initial time helps us to disentangle the sources of non-Gaussianity.

The functions J and K , given by equations (5), constrain the velocity coefficients proportional to \dot{D} and \dot{E} and depend on the actual physical situation (a dot denotes a time derivative w.r.t. t). We give the general solution for D and E for generic initial conditions in appendix A. Here we report a particular compelling class since their resulting expressions are closely related to the “slaved” initial conditions in refs [23–27], and can thus be interpreted to be of the Zel’dovich type [28]. Since these slaved initial conditions require an initial velocity which is proportional to some acceleration, we think they model the nature of adiabatic fluctuations reasonably well. We require for this restricted class $D(t_0) = E(t_0) = 0$, $\dot{D}(t_0) = 2t_0/3$, and $\dot{E}(t_0) = 2t_0^3/21$, which leads to

$$\begin{aligned} D(t) &= [a(t) - 1] t_0^2, \\ E(t) &= \left[-\frac{3}{7} a^2(t) + a(t) - \frac{4}{7} \right] t_0^4, \end{aligned} \quad (7)$$

for eq. (3). The fastest growing modes in D and E do not change for any choice of initial conditions but the decaying modes do. Our conclusions do not change for any other realistic initial conditions and hence our findings do not depend on the specific choice of the decaying modes in (7); we make this choice to be concrete in what follows. Our final results are also valid for Λ CDM.

III. NEWTONIAN COORDINATES AND THE DISPLACEMENT FIELD

To obtain a description in terms of the motion of particles we transform the result of the gradient expansion from the comoving coordinates (t, \mathbf{q}) to another coordinate system (τ, \mathbf{x}) . These two frames are connected by

¹ The Weyl tensor vanishes in three dimensions so the Riemann tensor is fully described in terms of the Ricci tensor.

² The same metric up to a transverse traceless tensor and without the decaying modes can also be found in equation (3.42) of [22].

the coordinate transformation

$$\begin{aligned} x_i(t, \mathbf{q}) &= q_i + \psi_i(t, \mathbf{q}) \\ \tau(t, \mathbf{q}) &= t + \mathcal{L}(t, \mathbf{q}), \end{aligned} \quad (8)$$

where ψ_i and \mathcal{L} are supposed to be small perturbations. We shall soon identify ψ and \mathcal{L} as the displacement field and its velocity potential, respectively. We thus transform the metric

$$ds^2 = -dt^2 + \gamma_{ij}(t, \mathbf{q}) dq^i dq^j, \quad (9)$$

to a Newtonian frame

$$\begin{aligned} ds^2 &= -[1 + 2A(\tau, \mathbf{x})] d\tau^2 \\ &\quad + a^2(\tau) [1 - 2B(\tau, \mathbf{x})] \delta_{ij} dx^i dx^j, \end{aligned} \quad (10)$$

where A, B are supposed to be small perturbations and γ_{ij} is given in equation (3). Note that we have neglected the excitation of vector and tensor modes. This can be straightforwardly rectified if needed. The coordinate transformation requires:

$$\begin{aligned} \gamma_{ij}(t, \mathbf{q}) &= -\frac{\partial \tau}{\partial q^i} \frac{\partial \tau}{\partial q^j} [1 + 2A(\tau, \mathbf{x})] \\ &\quad + a^2(\tau) \frac{\partial x^l}{\partial q^i} \frac{\partial x^m}{\partial q^j} \delta_{lm} [1 - 2B(\tau, \mathbf{x})], \end{aligned} \quad (11)$$

$$\begin{aligned} 0 &= -\frac{\partial \tau}{\partial t} \frac{\partial \tau}{\partial q^i} [1 + 2A(\tau, \mathbf{x})] \\ &\quad + a^2(\tau) \frac{\partial x^l}{\partial t} \frac{\partial x^m}{\partial q^i} \delta_{lm} [1 - 2B(\tau, \mathbf{x})], \end{aligned} \quad (12)$$

$$\begin{aligned} -1 &= -\frac{\partial \tau}{\partial t} \frac{\partial \tau}{\partial t} [1 + 2A(\tau, \mathbf{x})] \\ &\quad + a^2(\tau) \frac{\partial x^l}{\partial t} \frac{\partial x^m}{\partial t} \delta_{lm} [1 - 2B(\tau, \mathbf{x})]. \end{aligned} \quad (13)$$

We solve these equations for ψ , \mathcal{L} , A and B order by order. Formally, each small quantity is expanded in a series, i.e. $A = \epsilon A^{(1)} + \epsilon^2 A^{(2)} + \dots$, where ϵ is supposed to be a small dimensionless parameter. The primordial potential Φ is of order ϵ .

We report the results for the metric coefficients A and B in appendix B since they are not needed in the following. The coordinate transformation (8)—valid for arbitrary initial conditions but restricted to an EdS universe, is up to second order

$$\begin{aligned} x_i(t, \mathbf{q}) &= q_i + \frac{3}{2} D \Phi_{,i} + \left(\frac{3}{2}\right)^2 E \frac{\partial q_i}{\partial \mathbf{q}^2} \mu_2 \\ &\quad - 5D \partial_{q_i} \Phi^2 + \left[5D + \left(\frac{v}{a}\right)^2\right] \frac{\partial q_i}{\partial \mathbf{q}^2} C_2, \end{aligned} \quad (14)$$

where we can easily read off the displacement field ψ

according to (8), and

$$\begin{aligned} \tau(t, \mathbf{q}) &= t + v \Phi + \left(\frac{3}{2}\right)^2 a^2 \left[\frac{\dot{D} D}{2} \Phi_{,l} \Phi_{,l} + \dot{E} \frac{1}{\nabla_{\mathbf{q}}^2} \mu_2 \right] \\ &\quad + v \left[vH + \frac{3}{4} a^2 \ddot{D} - \frac{5}{3} \right] \Phi^2 \\ &\quad + v \left[2vH + 3a^2 \ddot{D} + \frac{10}{3} \right] \frac{1}{\nabla_{\mathbf{q}}^2} C_2, \end{aligned} \quad (15)$$

where a dot denotes a time derivative w.r.t. t , the Hubble parameter for an EdS universe is $H = 2/(3t)$, and we have defined

$$\mu_2 \equiv \frac{1}{2} (\Phi_{,ll} \Phi_{,mm} - \Phi_{,lm} \Phi_{,lm}), \quad (16)$$

$$v \equiv \frac{3}{2} a^2 \dot{D}, \quad (17)$$

$$C_2 \equiv \frac{1}{\nabla_{\mathbf{q}}^2} \left[\frac{3}{4} \Phi_{,ll} \Phi_{,mm} + \Phi_{,m} \Phi_{,lm} + \frac{1}{4} \Phi_{,lm} \Phi_{,lm} \right], \quad (18)$$

with $1/\nabla_{\mathbf{q}}^2$ being the inverse Laplacian.

Interestingly although not directly apparent, the kernel (18) has been also derived in ref [20] where the α of their eq. (18) is given by $\alpha \equiv -4\nabla_{\mathbf{q}}^{-2} C_2$. In [20] α arises in the evolution equation of the second-order curvature perturbation in the Poisson gauge.

The first line in eq. (14) agrees with Newtonian LPT [11, 25, 29, 30]; it contains the Zel'dovich approximation with its second-order improvement (2LPT). The remnant terms are relativistic corrections which should not bear much influence on the particle trajectories at late times. At initial time, however, they lead to an initial displacement and thus to a density perturbation. Also note that the time perturbations in the first line of eq. (15) correspond to the velocity perturbations in the Newtonian approximation. Indeed, v in the first line is the time coefficient of the velocity potential at leading order in LPT, and the bracketed term in the same line in eq. (15) leads to $\propto g(t) \nabla_{\mathbf{x}}^{-2} G_2$ in an Eulerian coordinate system, with

$$G_2 = \frac{3}{7} \Phi_{,ll} \Phi_{,mm} + \Phi_{,l} \Phi_{,lmm} + \frac{4}{7} \Phi_{,lm} \Phi_{,lm}, \quad (19)$$

which is the second-order kernel for the peculiar velocity in Newtonian perturbation theory [11]. The remnant terms in (15) are again absent in Newtonian LPT.

The precise choice of the decaying modes in D and E is of no great importance, reflecting only the chosen initial conditions [27]. However, it is very important to recognize the disappearance of the Newtonian part of the displacement field in (14) for $t \rightarrow t_0$ which occurs for *any* set of decaying modes. On the other hand, the last relativistic term in (14) is in general non-vanishing for $t \rightarrow t_0$. It generates the initial displacement (we additionally take the divergence of the very equation)

$$\lim_{t \rightarrow t_0} \nabla_{\mathbf{q}} \cdot [\mathbf{x}(t, \mathbf{q}) - \mathbf{q}] \equiv v_0^2 C_2, \quad (20)$$

with

$$v_0^2 = \left(\frac{3}{2} \frac{\partial D(t)}{\partial t} \right)^2 \Big|_{t=t_0}. \quad (21)$$

For our simplified initial conditions, i.e., with the use of the growth functions (7) we have $v_0^2 \rightarrow t_0^2$. The time derivative of D is proportional to a velocity potential since D is the time coefficient of the displacement. Thus, the above expression vanishes only if the initial velocity between the synchronous and Newtonian frame vanishes; this initial data however would be unphysical since we already specified a vanishing displacement field. On the contrary, for a non-zero initial velocity the displacement kernel (18) is enhanced.

Note again that the only restriction we have made to derive eq. (20) is to require $\gamma_{ij}(t_0, \mathbf{q}) = k_{ij}$ initially. In a Newtonian treatment, i.e., a coordinate transformation which relates two Euclidean metrics, the requirement of $\gamma_{ij}^{\text{Euclidean}}(t_0, \mathbf{q}) = k_{ij}$ would imply an exact overlapping of the Eulerian and Lagrangian frames at initial time. Expression (20) would thus vanish.

The above result is a purely relativistic effect. It results from the space-time mixing in the coordinate transformation (11). Note that eq. (20) is also valid for Λ CDM with the corresponding $D(t)$.

IV. OPTION A: INITIAL NON-GAUSSIANITY

The non-vanishing (relativistic) displacement field at initial time generates a density perturbation, which we shall use in the following to feed back to the Gaussian field:

$$\lim_{\tau \rightarrow t_0} \delta_{\Phi}^{(2)} \equiv -v_0^2 C_2(\mathbf{q}) - \frac{v_0 t_0}{2} T_1 \nabla_{\mathbf{q}}^2 \Phi^2, \quad (22)$$

with $T_1 = -(1 + 10c_1/(3t_0^{5/3}))$ and where c_1 is a constant which depends on the chosen initial conditions ($c_1 \rightarrow 0$ and so $T_1 \rightarrow -1$ for the above mentioned simplified initial conditions, see appendix A). The overall minus sign is the result of mass conservation. The last term in eq. (22) is the result of using the Newtonian time τ and taking the limit $\tau \rightarrow t_0$ for the relativistic trajectory (14) with the use of the time perturbation (15).

In Fourier space eq. (22) becomes

$$\begin{aligned} \tilde{\delta}_{\Phi}^{(2)}(\mathbf{k}) &= \frac{1}{4} \int \frac{d^3 k_1}{(2\pi)^3} \int \frac{d^3 k_2}{(2\pi)^3} (2\pi)^3 \delta_D^{(3)}(\mathbf{k}_{12} - \mathbf{k}) \\ &\quad \times F_{\text{NL}}(\mathbf{k}_1, \mathbf{k}_2) \tilde{\Phi}(\mathbf{k}_1) \tilde{\Phi}(\mathbf{k}_2), \end{aligned} \quad (23)$$

where we have defined the (already symmetrised) non-local kernel

$$F_{\text{NL}}(\mathbf{k}_1, \mathbf{k}_2) = 4v_0^2 [F_{\text{NL}}^{\text{STM}}(\mathbf{k}_1, \mathbf{k}_2) + F_{\text{NL}}^{\text{TP}}(\mathbf{k}_1, \mathbf{k}_2)], \quad (24)$$

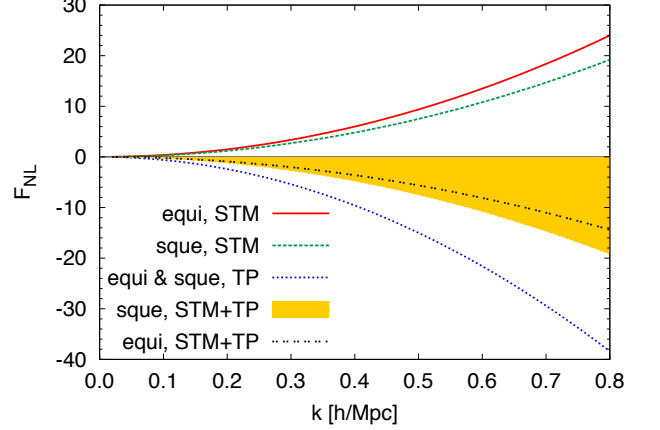


FIG. 1. Initial non-Gaussianity for the bispectrum (28) for different triangle configurations with $\mathbf{k}_{123} = \mathbf{0}$. We use the simplified initial conditions (with the respective growth functions (7)), and choose a redshift $z = 50$ such that $ct_0 \rightarrow 5.5 \text{ Mpc}/h$. We plot the individual expressions in F_{NL} given in eq. (24), taking into account the non-Gaussian power induced through space-time mixing (STM) and through the time-perturbation (TP). The red (solid) curve corresponds to an equilateral triangle with $k = k_1 = k_2 = k_3$. The green (dashed) curve denotes a squeezed triangle with $\Delta k = 0.012h/\text{Mpc}$ and $k = k_1 = k_2$. The blue (dotted) curve denotes the contribution through the time-perturbation and is identical for both squeezed and equilateral triangles. The yellow (shaded) region specifies the total amount, STM+TP, of non-Gaussianity for squeezed configurations, and the black (double dotted) curve is the total amount of non-Gaussianity for equilateral triangles.

where the kernels induced through space-time mixing (STM) and through the time perturbation (TP) are respectively

$$F_{\text{NL}}^{\text{STM}}(\mathbf{k}_1, \mathbf{k}_2) = \left(\frac{k_1 k_2}{k_{12}} \right)^2 \left[\frac{3}{4} + \frac{1}{2} \frac{\mathbf{k}_1 \cdot \mathbf{k}_2}{k_1 k_2} \left(\frac{k_1}{k_2} + \frac{k_2}{k_1} \right) + \frac{1}{4} \frac{(\mathbf{k}_1 \cdot \mathbf{k}_2)^2}{k_1^2 k_2^2} \right], \quad (25)$$

$$F_{\text{NL}}^{\text{TP}}(\mathbf{k}_1, \mathbf{k}_2) = \frac{t_0}{2v_0} T_1 k_{12}^2. \quad (26)$$

We use the short-hand notation $\mathbf{k}_{12} = \mathbf{k}_1 + \mathbf{k}_2$ and $k_{12} = |\mathbf{k}_{12}|$. With $\tilde{\delta}_{\Phi}^{(1)} = 2\Phi$ (see the following section) we have

$$\tilde{\delta}_{\Phi} = \tilde{\delta}_{\Phi}^{(1)} + \tilde{\delta}_{\Phi}^{(2)}, \quad (27)$$

and we recognize that the bispectrum induced through STM and TP is

$$B_{\Phi}(k_1, k_2, k_3) = 2F_{\text{NL}}(\mathbf{k}_1, \mathbf{k}_2) P_{\Phi}(k_1) P_{\Phi}(k_2) + \text{two permutations}, \quad (28)$$

at leading order, with the power spectrum

$$\langle \tilde{\Phi}(\mathbf{k}_1) \tilde{\Phi}(\mathbf{k}_2) \rangle_c \equiv (2\pi)^3 \delta_D^{(3)}(\mathbf{k}_{12}) P_\Phi(k_1), \quad (29)$$

and similarly for the bispectrum. In the following we compare F_{NL} from eq. (28) with the $f_{\text{NL}}^{\text{loc}}$ parameter from the primordial non-Gaussianity of the local type. In fig. 1 we plot the dimensionless quantity F_{NL} . We have used the simplified set of initial conditions, with growth functions given in (7). We have specified the initial time t_0 at a redshift z according to

$$t_0(z) \simeq \frac{2}{3H_{\text{today}}(1+z)^{3/2}}, \quad (30)$$

for an EdS universe, where $H_{\text{today}} = 100 \text{ km s}^{-1} h \text{ Mpc}^{-1}$, and h is the dimensionless Hubble parameter of order 0.7. We have fixed $z = 50$ in the figure³ but any other starting point is appropriate and just leads to a rescaling of the y -axis with the amplitude of F_{NL} getting smaller with larger z . In this figure we show the results for equilateral and squeezed triangles ($\Delta k = 0.012h/\text{Mpc}$). We have separated the non-Gaussian amplitude with respect to its origin, i.e., the amplitude from space-time mixing (STM) and from the time perturbation (TP). The yellow (shaded) region denotes the “sum” of both amplitudes for squeezed triangle configurations. Note that for squeezed triangles the amplitudes STM and TP are not partially summing/canceling itself as it is the case for equilateral triangles (which is denoted by the black [double dotted] curve). Instead, the kernel $F_{\text{NL}}^{\text{TP}}(\mathbf{k}_1, \mathbf{k}_2)$ is vanishing for $k_1 = k_2$ and $\mathbf{k}_1 + \mathbf{k}_2 + \Delta\mathbf{k} = \mathbf{0}$, and non-zero otherwise; this behaviour is reversed for the kernel $F_{\text{NL}}^{\text{STM}}$.

Equation (28) does only include the density perturbation induced through STM and TP (cf. eq. (22)). It is important to keep in mind that the initial acceleration between the frames (i.e., an initial acceleration of the particle) will induce a density perturbation as well—due to Einstein’s equivalence principle. The appearance of an initial acceleration obviously depends on the chosen initial conditions.

A precise scheme to implement this non-Gaussian component into an N -body simulation can be found in ref [31, 32]. Then, the displacement and the velocity of the particles is just with respect to the Newtonian trajectory, i.e., it is given by Newtonian 2LPT [33].

V. OPTION B: RELATIVISTIC TRAJECTORY

Here we include the relativistic corrections in the so-called active approach. We call it active since not the Gaussian field is modified as in the passive approach but the initial displacement of the particles.

The standard procedure to generate initial conditions in N -body simulation is to use Newtonian 2LPT [33, 34]. In there, particles are usually displaced according to the fastest growing mode solutions of the second-order displacement field together with its velocity field. Whilst incorporating relativistic corrections, however, one should include decaying modes as well, since they have roughly the same signature as the relativistic corrections. Additionally and crucially, by neglecting the decaying modes one loses the control to adjust the initial velocities of the particles. As a consequence the magnitude of the initial velocity is rather accidental if decaying modes are neglected (since the initial velocity is then given by time differentiating of the fastest growing mode only). The resulting statistics of the matter fields are accidental as well, so artificial transients could flaw the (initial) gravitational evolution. In appendix A we report the most general solution to adjust any initial data, depending on the actual physical situation. Here we describe how to set up generic initial data with the inclusion of (to be fixed) decaying modes together with the relativistic corrections. As before we require $D(t_0) = E(t_0) = 0$. Note that this requirement does not harm the initial density configuration as long as the velocity and the acceleration field is generated according to the full displacement field.

Suppose we have a simple rectangular grid in our N -body setting, thus without any spatial deformations. We adjust a universal clock which may be identified with an observers clock. We identify the universal clock to be τ , given in eq. (15). Then, the particles position (14) is given by the initial grid position $\mathbf{q}_{(i,j,k)} \equiv \mathbf{q}$ plus the displacement at initial time (we suppress the i, j, k label for the specific grid points):

$$\lim_{\tau \rightarrow t_0} x_i(\tau, \mathbf{q}) = q_i - \frac{v_0 t_0}{2} \left(1 + \frac{10}{3} \frac{c_1}{t_0^{5/3}} \right) \partial_i \Phi^2 + v_0^2 \frac{\partial_i}{\nabla_q^2} C_2, \quad (31)$$

where c_1 is a constant which depends on the chosen initial conditions (see appendix A). This is the initial displacement of the particles from its original unperturbed grid positions. Note that at initial time the above can be either evaluated at the vicinity of the Eulerian or Lagrangian spatial coordinate. This is however not true for the Eulerian and Lagrangian time. The velocity field at initial time is thus

$$\begin{aligned} u_i(t_0) &\equiv \lim_{\tau \rightarrow t_0} \frac{dx_i(\tau, \mathbf{q})}{d\tau} \\ &= v_0 \Phi_{,i} + \left(\frac{3}{2} \right)^2 E' \frac{\partial_i}{\nabla_q^2} \mu_2 \\ &\quad - \left[\frac{17}{3} v_0 + t_0 - \frac{20}{9} \frac{c_1}{t_0^{2/3}} \right] \partial_i \frac{\Phi^2}{2} \\ &\quad + \frac{4v_0}{3} \left[2 + \frac{v_0}{t_0} - 10c_1 t_0^{-5/3} \right] \frac{\partial_i}{\nabla_q^2} C_2, \quad (32) \end{aligned}$$

³ At $z = 158$ we have $ct_0 \rightarrow 1 \text{ Mpc}/h$.

where a prime denotes a differentiation with respect to Eulerian/Newtonian time τ .

Since we require a vanishing Newtonian displacement field at initial time we should specify the initial acceleration field for the sake to get a physical set of initial data. The obvious way to do so in an N -body simulation is simply to require an initial acceleration component for each CDM particle. Instead of that one can take use of Einstein's equivalence principle and translate the acceleration component into a density perturbation, i.e., allow different particle masses at different grid points. We report the required density perturbation in the following section.

It is then straightforward to include the above into N -body simulations. The general procedure how to obtain the displacement with its velocity on a grid can be found in appendix D2 in ref [33].

VI. THE DENSITY CONTRAST IN THE NEWTONIAN FRAME

For the sake of completeness we also derive the density contrast in the new coordinate system. In the following it is convenient to restrict to the fastest growing modes only, since then we have a clean identification with the density contrast from the (Newtonian) literature. The spatial transformation of the fastest growing mode is

$$x_+^i(t, \mathbf{q}) = q^i + \frac{3}{2}a(t)t_0^2\partial^i\Phi(t, \mathbf{q}) + \partial^i\psi_+^{(2)}(t, \mathbf{q}), \quad (33)$$

with the scalar

$$\psi_+^{(2)} = -\left(\frac{3}{2}\right)^2 \frac{3}{7}a^2t_0^4 \frac{1}{\nabla_q^2}\mu_2 - 5at_0^2\Phi^2 + 6at_0^2 \frac{1}{\nabla_q^2}C_2, \quad (34)$$

and the temporal transformation is

$$\tau_+(t, \mathbf{q}) = t + t\Phi(t, \mathbf{q}) + tL_+^{(2)}(t, \mathbf{q}), \quad (35)$$

with

$$L_+^{(2)}(t, \mathbf{q}) = \frac{3}{4}at_0^2\Phi_{,l}\Phi_{,l} - \frac{9}{7}at_0^2 \frac{1}{\nabla_q^2}\mu_2 - \frac{7}{6}\Phi^2 + 4\frac{1}{\nabla_q^2}C_2. \quad (36)$$

Note that the dependences in expressions (34) and (36) are either (t, \mathbf{q}) or (τ, \mathbf{x}) at second order. The energy density ρ for an EdS universe written in the synchronous gauge is [13]

$$\rho(t, \mathbf{q}) \equiv \bar{\rho}(t) [1 + \delta(t, \mathbf{q})] = \frac{3H_0^2}{8\pi G} \frac{[1 + \frac{10}{3}\Phi(\mathbf{q})]^{3/2}}{\sqrt{\det[\gamma_{ij}(t, \mathbf{q})]}}, \quad (37)$$

where $\bar{\rho}$ is the mean density. We thus transform the above according to (33) and (35). Then, we obtain the

density contrast in the Newtonian coordinate system:

$$\frac{\delta\rho(\tau, \mathbf{x})}{\bar{\rho}} = \delta^{(1)}(\tau, \mathbf{x}) + \delta^{(2)}(\tau, \mathbf{x}), \quad (38)$$

where

$$\delta^{(1)}(\tau, \mathbf{x}) = \delta_N^{(1)} + 2\Phi, \quad (39)$$

$$\delta^{(2)}(\tau, \mathbf{x}) = \delta_N^{(2)} + \frac{15}{4}at_0^2\Phi_{|l}\Phi_{|l} + 3at_0^2\Phi\Phi_{|l} - 3at_0^2 \frac{1}{\nabla_x^2}G_2 + 8\frac{1}{\nabla_x^2}C_2, \quad (40)$$

G_2 is given in equation (19), and the Newtonian part of the densities at first and second-order are respectively

$$\delta_N^{(1)}(\tau, \mathbf{x}) \equiv -\frac{3}{2}at_0^2\Phi_{|l}, \quad \delta_N^{(2)}(\tau, \mathbf{x}) \equiv \left(\frac{3}{2}\right)^2 a^2t_0^4 F_2, \quad (41)$$

with

$$F_2 = \frac{5}{7}\Phi_{|l}\Phi_{|lmm} + \Phi_{|l}\Phi_{|lmm} + \frac{2}{7}\Phi_{|lm}\Phi_{|lm}. \quad (42)$$

All dependences are w.r.t. (τ, \mathbf{x}) , a vertical slash $|_i$ denotes a partial derivative w.r.t. Eulerian coordinate x_i , and we have neglected terms $\propto \Phi^2$ which are not enhanced by spatial gradients. It is also interesting to note the following relation:

$$\frac{3}{2} \frac{1}{\nabla_x^2} G_2 = \frac{3}{2} C_2 - \left(\frac{3}{2}\right)^2 \frac{3}{7} \frac{1}{\nabla_x^2} \mu_2. \quad (43)$$

It links the second-order velocity perturbation to the second-order displacement field—through C_2 . Thus, a term $\propto at_0^2 C_2$ also arises in the density contrast (40). Its prefactor differs though in comparison with eq. (22) since we neglect decaying modes in this section but also since it is derived in a different gauge.

Our result (38) seems to be in agreement with the second-order density contrast in the Poisson gauge in ref [20], i.e., we obtain the same spatial functions after a couple of manipulations. However, the prefactors seem to disagree. We leave the full analytic comparison of the second-order δ in eq. (29) of ref [20] for a future project.

VII. WHICH DENSITY IS MEASURED IN NEWTONIAN N -BODY SIMULATIONS?

In sections IV and V we have formulated two ways how to include the relativistic corrections. Both could be incorporated whilst setting up the initial conditions in N -body simulations. In the last section we have calculated the density contrast in the Newtonian gauge, so one might wonder which density will be measured in N -body simulations. Since we assume that the onwarding gravitational evolution in such simulations is still performed on a rectangular grid, the density contrast will be the

same as in the Newtonian approximation. If the simulation could entirely satisfy general relativity we would measure the density contrast in the Newtonian gauge. This is so since space-time is deformed in general relativity and so is its 3-volume. Thus, to measure the (mass) density in the Newtonian gauge, eq. (38), we have to deform the volume V_G of the grid cells in the N -body simulation according to

$$V_G(t) = \int_G J d^3q, \quad (44)$$

with the peculiar Jacobian [24, 35]

$$J := \sqrt{\det[g_{ij}]/\det[k_{ij}]}, \quad g_{ij} := k_{ab} x^a_{,i} x^b_{,j}, \quad (45)$$

where the second-order deformation tensor $x_{i,j}$ is given by partial differentiation of eq. (14). The local density in the Newtonian gauge is then just the ratio of massive particles in the grid cell to the deformed volume V_G .

VIII. CONCLUSIONS

We obtained the relativistic Lagrangian displacement field together with its velocity potential from a general relativistic gradient expansion for an Einstein-de Sitter universe. By requiring that the metric reduces to a given initial condition in the synchronous comoving/Lagrangian frame we found a non-zero initial displacement field in the Newtonian/Eulerian frame which is absent in a purely Newtonian description. This initial displacement depends on the initial velocity potential of the particle, at second order in the primordial potential. We gave an example of initial conditions which are closely related to the so-called “slaved” ones and are thus of the Zel’dovich type. By including the decaying modes in the growth functions, we report the most general solution for the displacement and velocity in appendix A.

The findings allow us to study the relevance of the velocity (of the fluid particle) between the synchronous and Newtonian coordinate system. We find that an initial velocity between the frames generates a non-local density perturbation. This is a purely relativistic effect which originates from two distinct sources, (1) space-time mixing in the coordinate transformation (11), and (2) from the fact that the particles’ proper time is coordinate dependent. The net effect is not a result of the gravitational non-linear evolution, and it is even apparent if the

initial acceleration is zero. (Non-zero accelerations generate density perturbations even in the Newtonian treatment.) Equation (28) shows that the coordinate transformation induces a small velocity dependent amount of non-Gaussianity whose scale-dependence is depicted in fig. 1. Our result could be of importance in situations where the velocities of the traced objects are relatively high, since the f_{NL} amplitude depends on the particle velocity potential squared.

We considered the generation of initial conditions in N -body simulations which we described in section IV: Instead of using the relativistic trajectory (14) one can treat the relativistic corrections in terms of an initial non-Gaussianity component, which acts as a correction to the (Lagrangian) potential and thus as a correction to the initial Gaussian field. We therefore adjust the cosmological potential with respect to the initial non-local density perturbation but then let the particles evolve according to the Newtonian trajectory. This establishes a simple quasi-relativistic N -body simulation, and we call it the passive approach. In section V we described the active approach—the alternative way to incorporate the relativistic corrections in N -body simulations. In the active approach, the initial Gaussian field is unaltered but the particle trajectories include relativistic corrections. As an important note, we assume that the resulting initial statistics in both approaches are equivalent, leave however the cumbersome proof for future work. If the resulting statistics agree, the same Lagrangian method could be used to generate non-Gaussian initial conditions for purely Newtonian N -body simulations.

Finally, in section VII we showed how to relate the density contrast from N -body simulations to the one in the Newtonian gauge. Essentially, space-time is deformed and so is the 3-volume of the grid cells. Thus, the density in the Newtonian gauge is obtained by relating it to the appropriate physical volume.

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Appendix A: General growth functions

The general solutions for the displacement coefficients (4) in an EdS universe are

$$D(t) = \left[t^{2/3} - \frac{20}{9} \frac{c_1}{t} + \frac{20}{9} c_2 \right] t_0^{4/3}, \quad (\text{A1})$$

$$E(t) = \left[-\frac{3}{7} t^{4/3} - \frac{20}{9} c_2 t^{2/3} - \frac{40}{9} \frac{c_1}{t^{1/3}} - \frac{200}{81} \frac{c_3}{t} + \frac{400}{81} \frac{c_1 c_2}{t} - \frac{100}{81} \frac{c_1^2}{t^2} + \frac{200}{81} c_4 \right] t_0^{8/3}, \quad (\text{A2})$$

where $c_1 - c_4$ are constants. To fix the constants one may choose specific initial data for $D(t_0)$ and $E(t_0)$ together with its first time derivatives. Again, this conforms to specify the initial displacement and the initial velocity.

Generally it could be also appropriate to fix the initial peculiar gravitational field instead of the initial velocity, since the former sources a density perturbation and thus could flaw our main argument in this paper (i.e., that the initial non-Gaussianity is sourced only through initial velocity perturbations). Indeed, defining the time coefficient of the initial peculiar gravitational field as

$$g_{\text{pec}}(t_0) = \frac{4}{3t_0} \dot{D}(t_0) + \ddot{D}(t_0), \quad (\text{A3})$$

up to first order (similarly for the higher order coefficients), we can construct displacements which are entirely without initial accelerations. We call this initial data “inertial”, and the resulting displacement coefficients are then

$$D_{\text{inert}}(t) = \left[a - a^{-3/2} \right] t_0^2, \quad (\text{A4})$$

$$E_{\text{inert}}(t) = \left[-\frac{3}{7} a^2 - 2a^{-1/2} + \frac{75}{28} a^{-3/2} - \frac{1}{4} a^{-3} \right] t_0^4. \quad (\text{A5})$$

As can be proven by direct verification, the above modes do not change our conclusions: the coordinate transformation yields to a density perturbation which is only sourced by a velocity perturbation.

Appendix B: Perturbations in the Newtonian metric

Here we summarise our findings for the metric

$$ds^2 = -[1 + 2A(\tau, \mathbf{x})] d\tau^2 + a^2(\tau) [1 - 2B(\tau, \mathbf{x})] \delta_{ij} dx^i dx^j. \quad (\text{B1})$$

To avoid cumbersome expressions we restrict to an EdS universe and take only the fastest growing modes into account. Up to second order in Φ the metric coefficients are

$$A(\tau, \mathbf{x}) \simeq \phi_{\text{N}} - \phi_{\text{R}}, \quad (\text{B2})$$

and

$$B(\tau, \mathbf{x}) \simeq \phi_{\text{N}} + \frac{2}{3}\phi_{\text{R}}, \quad (\text{B3})$$

with

$$\phi_{\text{N}} = -\Phi + \frac{3}{4}a(\tau)t_0^2\Phi_{|l}\Phi_{|l} + \frac{15}{7}a(\tau)t_0^2\frac{1}{\nabla_{\mathbf{x}}^2}\bar{\mu}_2, \quad (\text{B4})$$

$$\phi_{\text{R}} = \frac{4}{\nabla_{\mathbf{x}}^2\nabla_{\mathbf{x}}^2} \left[\frac{3}{4}\Phi_{|l}\Phi_{|mm} + \Phi_{|l}\Phi_{|lmm} + \frac{1}{4}\Phi_{|lm}\Phi_{|lm} \right], \quad (\text{B5})$$

$$\bar{\mu}_2 = \frac{1}{2}(\Phi_{|ll}\Phi_{|mm} - \Phi_{|lm}\Phi_{|lm}). \quad (\text{B6})$$

A vertical slash “ $|_i$ ” denotes a differentiation w.r.t. Eulerian coordinate x_i . Note that we have $\Phi \equiv \Phi(t_0, \mathbf{x})$

for this appendix. The term ϕ_{N} can be obtained from a purely Newtonian treatment [17, 36], and it is just the cosmological potential up to second order. Indeed, multiplying the second term on the RHS with $\nabla_{\mathbf{x}}^2/\nabla_{\mathbf{x}}^2$ we find

$$\phi_{\text{N}} = -\Phi + \frac{3}{2}a(\tau)t_0^2\frac{1}{\nabla_{\mathbf{x}}^2}F_2(t_0, \mathbf{x}), \quad (\text{B7})$$

with the well-known second-order kernel

$$F_2(t_0, \mathbf{x}) = \frac{5}{7}\Phi_{|ll}\Phi_{|mm} + \Phi_{|l}\Phi_{|lmm} + \frac{2}{7}\Phi_{|lm}\Phi_{|lm}. \quad (\text{B8})$$